Wigner formula of rotation matrices and quantum walks

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Quantization of a random-walk model is performed by giving a multi-component qubit to a walker at site and by introducing a quantum coin, which is represented by a unitary matrix. In quantum walks, the qubit of walker is mixed according to the quantum coin at each time step, when the walker hops to other sites. The standard (discrete) quantum-walk model in one-dimension is defined by using a 2×2 unitary matrix for a walker with two-component qubit. In this paper we use Wigner's $(2j+1)$-dimensional unitary representations of rotations as quantum coins, where j is a half-integer, and introduce a family of one-dimensional quantum walks with $(2j+1)$-component qubits. For any value of half-integer j, convergence of all moments of walker's pseudovelocity in the long-time limit is proved. It is generally shown for the present models that, if $(2j+1)$ is even, the limit distribution is given by a superposition of $(2j+1)/2$ terms of scaled Konno's density functions, and if $(2j+1)$ is odd, it is a superposition of j terms of scaled Konno's density functions and a Dirac's delta function at the origin. For the two-, three-, and four-component models, the limit distribution functions are explicitly calculated and their dependence on the parameters of quantum coins and on the initial qubit of walker is completely determined. Comparison with computer simulation results is also shown.

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I. INTRODUCTION

No one doubts the importance of random-walk models in physics, mathematics and computer sciences. In particular, when we explain basic concepts of statistical physics [1], stochastic processes in physics and chemistry [2], and stochastic algorithms [3], introduction of random-walk models is very useful and effective. It is interesting to see that systematic study of quantization of random walks is not old [4, 5, 6, 7]. As expected, the study of quantum walks is fruitful and its results have been applied to solve the transport problems in solid-state physics of strongly correlated electron systems [8], to derive non-Gaussian-type central limit theorems in probability theory [9, 10, 11], and to invent new algorithms in the quantum information theory [12, 13]. The research field of quantum walks is growing widely [14, 15, 16] and mathematical understanding of the new models is becoming deeper [17, 18, 19, 20] in recent years.

It should be noted here that, from the view-point of standard quantum mechanics, "to quantize random walks" is a contradictory concept, since in quantum mechanics, time-evolution of a state vector $|\Psi(t)\rangle$, or a wave function $\Psi(x,t)$, is given by a deterministic unitary transformation associated with the Hamiltonian and probability concept appears in the theory only when we perform observation of physical quantities, *i.e.*, when we calculate the probability density $p(x,t) = |\Psi(x,t)|^2$ at a given time. On the other hand, random walk is a typical example of stochastic processes, in which we toss a coin to select a walk at each time step. In an earlier paper [21], it was shown that the one-dimensional standard random walk can be realized by a random-turn model [22], in which a coin is represented by a 2×2 stochastic matrix and that, if we replace the matrix by a 2×2 unitary matrix, a one-dimensional quantum-walk model is obtained. This argument is not only heuristic but also generic, since it implies that quantization of random-walk models can be done by introducing appropriate unitary matrices such that they play the roles of "quantum coins".

The consequence of this quantization procedure is the following. The obtained time-evolution of quantum walk is described by *multi-component* version of quantum-mechanical equation of motion. For the standard quantum-walk model on one-dimensional lattice $\mathbf{Z} = \{\cdots, -2, -1, 0, 1, 2, \cdots\}$ with the nearest-neighbor hopping, the equation is identified with the Weyl equation for two-component wave functions [21]. It should be remarked that such multi-component equations have been usually used in *relativistic* quantum mechanics [23].

In the present paper, we introduce a family of models of quantum walks on one-dimensional lattice $\mathbf{Z}$ indexed by a half-integer $j = 1/2, 1, 3/2, 2, \cdots$. As quantum coins, we use the $(2j+1)$-dimensional unitary representations of three-dimensional rotations $R^{(j)}(\alpha, \beta, \gamma)$, which are parameterized by three real numbers α, β, γ (the Euler angles) and are called the rotation matrices [24].

In our model with j and three parameters (α, β, γ), a quantum walker is assumed to be at the origin at time

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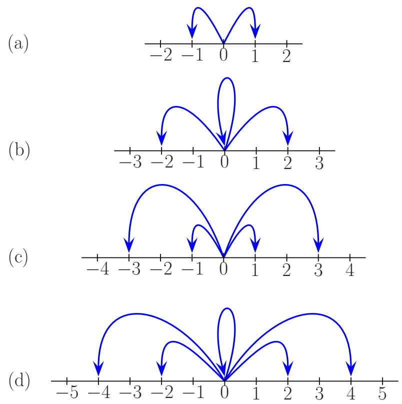

FIG. 1: Elementary hopping of quantum walker in the models with (a) $j = 1/2$ (two-component model), (b) $j = 1$ (three-component model), (c) $j = 3/2$ (four-component model), and (d) $j = 2$ (five-component model). When $(2j + 1)$ is odd, the walker can stay at the same position in a step, as shown by cyclic arrows at the origin in the cases (b) and (d).

$t = 0$ with a $(2j + 1)$-component qubit

$$\phi_0^{(j)} = \begin{pmatrix} q_j \\ q_{j-1} \\ \cdots \\ q_{-j+1} \\ q_{-j} \end{pmatrix} \quad \text{with} \quad \sum_{m=-j}^{j} |q_m|^2 = 1, \qquad (1)$$

where $q_m \in \mathbf{C}$(complex numbers), $m = -j, -j+1, \cdots, j$. At each time step $t = 1, 2, 3, \cdots$, the components of qubit are mixed according to a quantum coin $R^{(j)}(\alpha, \beta, \gamma)$ and the walker hops to $(2j + 1)$ sites on $\mathbf{Z}$, as illustrated by Fig.1 for $j = 1/2, 1, 3/2$ and 2 (see Eq. (15) below). When $j = 1/2$, $R^{(1/2)}(\alpha, \beta, \gamma)$ can be identified with an element of SU(2) appropriately parameterized by the three variables (the Cayley-Klein parameters) and the model is reduced to the standard two-component model [21]. It should be noted here that, when j is an integer (i.e. $(2j + 1)$ is odd), the walker can stay at the same position in a step.

Using the method of [11], we will prove that any moments of pseudovelocity of walker, which is defined by X_t/t (the position at time t, X_t, divided by t), converges in the long-time limit $t \to \infty$, and show that the limit distribution function is generally described by a superposition of appropriately scaled forms of a function

$$\mu(x; a) = \frac{\sqrt{1 - a^2}}{\pi(1 - x^2)\sqrt{a^2 - x^2}} \mathbf{1}_{\{|x|<|a|\}}, \qquad (2)$$

where $\mathbf{1}_{\{\omega\}}$ denotes the indicator function of a condition ω; $\mathbf{1}_{\{\omega\}} = 1$ if ω is satisfied and $\mathbf{1}_{\{\omega\}} = 0$ otherwise, and a is a real parameter. It is the density function first introduced by Konno to describe the limit distributions of the standard two-component quantum walks in his weak limit theorem [9, 10]. (As shown in Fig.2(a) in Sec.V, $\mu(x; a)$ is inversed bell-shaped on a finite support $x \in (-a, a)$ in big contrast with the Gaussian distribution, which describes the diffusion scaling limit of the classical random walks.) More precisely speaking, when $(2j+1)$ is even, the limit distribution function consists of $(2j+1)/2$ terms of Konno's density functions (2), and when $(2j+1)$ is odd, it does of j terms of Konno's and a point mass at the origin, which corresponds to the positive probability to retain the position of walker in a step (see Eq.(47)).

The weight functions $\mathcal{M}^{(j,m)}$ of these Konno's density functions (and the weight $\Delta^{(j)}$ of Dirac's delta function at the origin, when $(2j + 1)$ is odd) in the superposition depend on the parameters of quantum coin and the $(2j + 1)$ components of initial qubit (1) of quantum walker. We have found that the representation theory of groups [25] is useful to calculate the weight functions. Especially the Wigner formula for rotation matrices [24, 26] is critical. In this paper we give the explicit forms of weight functions for $j = 1/2, 1$ and $3/2$ (two-, three- and four-component models, respectively) and these results imply that the weight functions $\mathcal{M}^{(j,m)}$ are generally given by polynomials. Through these polynomials, the initial-qubit dependence of the limit distribution of pseudovelocity is completely determined.

This paper is organized as follows. In Sec.II, Wigner formula of $(2j+1)$-dimensional representation of the rotation group SO(3) is summarized. The family of quantum-walk models associated with the rotation matrices is defined for quantum walkers with $(2j+1)$-component qubit in Sec.III. Sec.IV is devoted to proving the generalized weak limit theorem (convergence of all moments) for pseudovelocities of quantum walks. There the polynomials, which give the weights of Konno's density functions and the point mass in the limit distributions, are listed for $j = 1/2, 1$ and $3/2$, explicitly. Comparison with computer simulation with the present analytic results is given in Sec.V. In this last section, we also discuss the relation between our results and previous multi-component models [27, 28, 29, 30] and possible future problems.

II. WIGNER FORMULA OF $(2j + 1)$-DIMENSIONAL REPRESENTATIONS OF ROTATION GROUP

Any rotation in the three-dimensional real space $\mathbf{R}^3$ is uniquely specified by three rotation angles α, β, γ called the Euler angles. In the quantum mechanics, the rotation with the Euler angles α, β, γ is given by an operator of the form (see, for instance, [24])

$$\hat{R}(\alpha, \beta, \gamma) = e^{-\mathrm{i}\alpha \hat{J}_3} e^{-\mathrm{i}\beta \hat{J}_2} e^{-\mathrm{i}\gamma \hat{J}_3}, \qquad (3)$$

where $\hat{\mathbf{J}} = (\hat{J}_1, \hat{J}_2, \hat{J}_3)$ is the vector operator of angular momentum, whose elements satisfy the su(2) Lie algebra,

$$[\hat{J}_k, \hat{J}_\ell] = \mathrm{i} \sum_{m=1}^{3} \varepsilon_{k\ell m} \hat{J}_m, \quad k, \ell = 1, 2, 3, \qquad (4)$$

with the completely antisymmetrical tensor with three indices $\varepsilon_{k\ell m}$ [25]. Let the ket-vector $|j, m\rangle, j =$

$0, 1/2, 1, 3/2, \cdots, m = -j, -j+1, \cdots, j$, denote the normalized eigenstates of $\hat{\mathbf{J}}^2 = \sum_{k=1}^3 \hat{J}_k^2$ and $\hat{J}_3$ such that $\hat{\mathbf{J}}^2|j,m\rangle = j(j+1)|j,m\rangle$, and $\hat{J}_3|j,m\rangle = m|j,m\rangle$. (We set $\hbar = 1$ in this paper.) Then, for each fixed value of half-integer j, a $(2j+1)\times(2j+1)$ unitary matrix $R^{(j)}(\alpha,\beta,\gamma) = (R^{(j)}_{mm'}(\alpha,\beta,\gamma))$ is defined with its elements

$$R^{(j)}_{mm'}(\alpha,\beta,\gamma) = \langle j,m|\hat{R}(\alpha,\beta,\gamma)|j,m'\rangle, \tag{5}$$

$m, m' = -j, -j+1, \cdots, j$.

We can show that

$$R^{(j)}_{mm'}(\alpha,\beta,\gamma) = e^{-\mathrm{i}\alpha m} r^{(j)}_{mm'}(\beta) e^{-\mathrm{i}\gamma m'} \tag{6}$$

with

$$r^{(j)}_{mm'}(\beta) = \sum_{\ell} \Gamma(j,m,m',\ell) \left(\cos\frac{\beta}{2}\right)^{2j+m-m'-2\ell} \left(\sin\frac{\beta}{2}\right)^{2\ell+m'-m}, \tag{7}$$

where

$$\Gamma(j,m,m',\ell) = (-1)^{\ell} \frac{\sqrt{(j+m)!(j-m)!(j+m')!(j-m')!}}{(j-m'-\ell)!(j+m-\ell)!\ell!(\ell+m'-m)!}. \tag{8}$$

In (7) the summation $\sum_\ell$ extends over all integers of ℓ for which the arguments of the factorials are positive or null ($0! = 1$). The matrix (6) gives a $(2j+1)$-dimensional irreducible representation of the rotation group SO(3) and is called the rotation matrix. Eq.(7) is known as the Wigner formula [24, 26]. In the present paper, when we write matrices and vectors whose elements are labeled by m, m', we will assume that the indices m and m' run from j to $-j$ in steps of -1. In Appendix A, we give explicit expressions of matrices $r^{(j)}(\beta) = (r^{(j)}_{mm'}(\beta))$ for $j = 1/2, 1$ and $3/2$.

III. QUANTUM-WALK MODELS WITH $(2j+1)$-COMPONENT QUBITS

Here we propose a new family of models of quantum walks on the one-dimensional lattice $\mathbf{Z}$, in which each walker has a $(2j+1)$-component qubit (1). In the previous paper [21], we reported the weak limit theorem for the two-component model. That model is generated by a quantum coin represented by a matrix in SU(2)

$$A = \begin{pmatrix} ue^{\mathrm{i}\theta} & \sqrt{1-u}e^{\mathrm{i}\phi} \\ -\sqrt{1-u^2}e^{-\mathrm{i}\phi} & ue^{-\mathrm{i}\theta} \end{pmatrix}, \quad u \in [-1,1],\ \theta,\phi \in [-\pi,\pi) \tag{9}$$

and a spatial shift-operator on $\mathbf{Z}$, which is represented by a matrix

$$S(k) = \begin{pmatrix} e^{\mathrm{i}k} & 0 \\ 0 & e^{-\mathrm{i}k} \end{pmatrix}, \quad k \in [-\pi,\pi) \tag{10}$$

in the wave-number space (k-space). If we compare these matrices with (6) with $j = 1/2$ and (A1) in Appendix A, we find that they are the special cases of $R^{(1/2)}(\alpha,\beta,\gamma)$;

$$\begin{aligned} A &= R^{(1/2)}(\pi-\theta-\phi, 2\arccos(u), -\pi-\theta+\phi), \\ S(k) &= R^{(1/2)}(-2k,0,0). \end{aligned} \tag{11}$$

From the view point of the group theory, we can give the following remark. In [21] we used the fact that SU(2)$\simeq \mathbf{S}^3$ ($\equiv$ the three dimensional unit sphere in $\mathbf{R}^4$) and the quantum coin A was parameterized by three real numbers, u, θ, ϕ (the Cayley-Klein parameters), corresponding the dimensionality 3 of the group space. On the other hand, we are now regarding the quantum coin A as a two-dimensional representation of the rotation group SO(3), and thus the three parameters are identified with the Euler angles for rotations in the three-dimensional real-space $\mathbf{R}^3$.

This observation had led us to adopt the $(2j+1)$-dimensional representation of the rotation group, $R^{(j)}(\alpha,\beta,\gamma)$, as a quantum coin to mix $(2j+1)$ components in qubit (1). The spatial shift-matrix is given by $S^{(j)}(k) = R^{(j)}(-2k,0,0) = \mathrm{diag}(e^{-2\mathrm{i}jk}, e^{-2\mathrm{i}(j-1)k}, \cdots, e^{2\mathrm{i}jk})$.

We assume at the initial time $t = 0$ that the walker is located at the origin. Then, in the k-space, the $(2j+1)$-component wave function of the walker at time t is given by

$$\hat{\Psi}^{(j)}(k,t) = \left(V^{(j)}(k)\right)^t \phi_0^{(j)}, \quad t = 0,1,2,\cdots, \tag{12}$$

where

$$\begin{aligned} V^{(j)}(k) &= V^{(j)}(k;\alpha,\beta,\gamma) \\ &\equiv S^{(j)}(k)R^{(j)}(\alpha,\beta,\gamma). \end{aligned} \tag{13}$$

The time evolution in the real space $\mathbf{Z}$ is then obtained by performing the Fourier transformation,

$$\begin{aligned}\Psi^{(j)}(x,t) &= \int_{-\pi}^{\pi}\frac{dk}{2\pi}\hat{\Psi}^{(j)}(k,t)e^{\mathrm{i}kx},\\ \hat{\Psi}^{(j)}(k,t) &= \sum_{x\in\mathbf{Z}}\Psi^{(j)}(x,t)e^{-\mathrm{i}kx},\end{aligned} \tag{14}$$

as

$$\Psi^{(j)}_m(x,t{+}1) = \sum_{m'=-j}^{j} R^{(j)}_{mm'}\Psi^{(j)}_{m'}(x{+}2m,t),\ t=0,1,2,\cdots, \tag{15}$$

where $\Psi^{(j)}_m(x,t)$ denotes the m-th component of the $(2j+1)$-component wave function $\Psi^{(j)}(x,t)$.

Now the stochastic process of $(2j{+}1)$-component quantum walk is defined on $\mathbf{Z}$ as follows. Let $X^{(j)}_t$ be the position of the walker at time t. The probability that we find the walker at site $x\in\mathbf{Z}$ at time t is given by

$$\mathrm{Prob}(X^{(j)}_t = x) = P(x,t) = [\Psi^{(j)}(x,t)]^{\dagger}\Psi^{(j)}(x,t), \tag{16}$$

where $[\Psi^{(j)}(x,t)]^{\dagger}$ is the hermitian conjugate of $\Psi^{(j)}(x,t)$. As shown in [21], the r-th moment of $X^{(j)}_t$ is given by, $r=0,1,2,\cdots$,

$$\begin{aligned}\langle (X^{(j)}_t)^r\rangle &\equiv \sum_{x\in\mathbf{Z}} x^r P(x,t)\\ &= \int_{-\infty}^{\infty}\frac{dk}{2\pi}[\hat{\Psi}^{(j)}(k,t)]^{\dagger}\left(\mathrm{i}\frac{d}{dk}\right)^{r}\hat{\Psi}^{(j)}(k,t).\end{aligned} \tag{17}$$

IV. LIMIT DISTRIBUTIONS OF QUANTUM WALKERS

A. Decomposition of time-evolution matrix

A key lemma for the following analysis of the quantum-walk models is the fact that the time-evolution matrix $V^{(j)}(k)$ defined by (13) is decomposed into the three rotation matrices $R^{(j)}$'s of the form

$$\begin{aligned}V^{(j)}(k) &= R^{(j)}(\phi(k),\theta(k),0)R^{(j)}(-p(k),0,0)\\ &\quad\times[R^{(j)}(\phi(k),\theta(k),0)]^{\dagger},\end{aligned} \tag{18}$$

where $\phi(k),\theta(k)$ and $p(k)$ are related with the Euler angles α,β,γ and the wave number k by

$$\begin{aligned}\frac{1}{2}\{(\alpha-2k)-\gamma\} &= \phi(k)+\frac{\pi}{2},\\ \tan\frac{1}{2}\{(\alpha-2k)+\gamma\} &= -\tan\frac{p(k)}{2}\cos\theta(k),\\ \sin\frac{\beta}{2} &= \sin\frac{p(k)}{2}\sin\theta(k).\end{aligned} \tag{19}$$

We give the proof of this formula in Appendix B.

The formula (18) means that the time-evolution matrix $V^{(j)}(k)$ can be diagonalized to $R^{(j)}(-p(k),0,0)$ by a unitary transformation given by $R^{(j)}(\phi(k),\theta(k),0)$. Indeed $R^{(j)}(-p(k),0,0)$ is a diagonal matrix $R^{(j)}(-p(k),0,0) = \mathrm{diag}(e^{\mathrm{i}jp(k)}, e^{\mathrm{i}(j-1)p(k)},\cdots,e^{-\mathrm{i}jp(k)})$ and, by the unitarity of $R^{(j)}$, $[R^{(j)}]^{\dagger}=[R^{(j)}]^{-1}$, (12) is written as

$$\begin{aligned}\hat{\Psi}^{(j)}(k,t) &= R^{(j)}(\phi(k),\theta(k),0)\begin{pmatrix} e^{\mathrm{i}tjp(k)} & & & \\ & e^{\mathrm{i}t(j-1)p(k)} & & \\ & & \ddots & \\ & & & e^{-\mathrm{i}tjp(k)}\end{pmatrix}[R^{(j)}(\phi(k),\theta(k),0)]^{\dagger}\phi^{(j)}_0\\ &= \sum_{m=-j}^{j} e^{\mathrm{i}tmp(k)}\mathbf{v}^{(j)}_m(k)C^{(j)}_m(k),\end{aligned} \tag{20}$$

where $\mathbf{v}^{(j)}_m(k)$ is the m-th column vector in the matrix $R^{(j)}(\phi(k),\theta(k),0)$,

$$\mathbf{v}^{(j)}_m(k) = \begin{pmatrix} R^{(j)}_{jm}(\phi(k),\theta(k),0)\\ R^{(j)}_{j-1\,m}(\phi(k),\theta(k),0)\\ \cdots\\ R^{(j)}_{-jm}(\phi(k),\theta(k),0)\end{pmatrix}$$

and

$$C^{(j)}_m(k) \equiv [\mathbf{v}^{(j)}_m(k)]^{\dagger}\phi^{(j)}_0 = \sum_{m'=-j}^{j}\overline{R^{(j)}_{m'm}}(\phi(k),\theta(k),0)q_{m'}, \tag{21}$$

where $\overline{z}$ denotes the complex conjugate of a complex number z.

The expansion (20) gives

$$\begin{aligned}&\left(\mathrm{i}\frac{d}{dk}\right)^{r}\hat{\Psi}^{(j)}(k,t)\\ &= \sum_{m=-j}^{j}\left(-m\frac{dp(k)}{dk}\right)^{r} e^{\mathrm{i}tmp(k)}\mathbf{v}^{(j)}_m(k)C^{(j)}_m(k)\,t^r\\ &\qquad +\mathcal{O}(t^{r-1}).\end{aligned}$$

Since $R^{(j)}$ is unitary, its column vectors make a set of orthonornal vectors, $[\mathbf{v}^{(j)}_m(k)]^{\dagger}\mathbf{v}^{(j)}_{m'}(k) = \delta_{mm'}$. Then we have

$$[\hat{\Psi}^{(j)}(k,t)]^\dagger \left(\mathrm{i}\frac{d}{dk}\right)^r \hat{\Psi}^{(j)}(k,t)$$
$$= \sum_{m=-j}^{j} \left(-m\frac{dp(k)}{dk}\right)^r |C_m^{(j)}(k)|^2 t^r + \mathcal{O}(t^{r-1}),$$

and thus (17) gives the following expression for moments of pseudovelocity $X_t^{(j)}/t$ in the long-time limit [11, 21],

$$\lim_{t\to\infty} \left\langle \left(\frac{X_t^{(j)}}{t}\right)^r \right\rangle$$
$$= \sum_{m:0<m\le j} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left\{(-1)^r |C_m^{(j)}(k)|^2 + |C_{-m}^{(j)}(k)|^2\right\}$$
$$\times \left(m\frac{dp(k)}{dk}\right)^r, \tag{22}$$

$r = 1, 2, 3, \cdots$, where the summation is taken over $m = 1/2, 3/2, \cdots, j$, if j is a half of odd number, and $m = 1, 2, \cdots, j$, if j is a positive integer. Here it should be noted that, when j is a positive integer, $m = 0$ mode exists, but it does not contribute to any moment of order $r = 1, 2, 3, \cdots$ in (22). The $m = 0$ mode comes from the fact that the walker can stay at the same position in a step, when $(2j + 1)$ is odd, and its contribution to the limit distribution will be described by a point mass at the origin (see Sec.IV.C).

B. Planar orbits in parameter space and integrals

The equations (19) define a one-parameter family (with parameter k) of transformations from the Euler angles (α, β, γ) to (p, θ, ϕ). More explicitly, we can find the following equations from (19) (see Appendix B),

$$\cos\frac{p(k)}{2} = \cos\frac{\beta}{2}\cos\frac{1}{2}(\alpha+\gamma-2k), \tag{23}$$
$$\sin\frac{p(k)}{2} = \sqrt{1-\cos^2(\beta/2)\cos^2\{(\alpha+\gamma-2k)/2\}}, \tag{24}$$
$$\cos\theta(k) = -\frac{\cos(\beta/2)\sin\{(\alpha+\gamma-2k)/2\}}{\sqrt{1-\cos^2(\beta/2)\cos^2\{(\alpha+\gamma-2k)/2\}}}, \tag{25}$$
$$\sin\theta(k) = \frac{\sin(\beta/2)}{\sqrt{1-\cos^2(\beta/2)\cos^2\{(\alpha+\gamma-2k)/2\}}}, \tag{26}$$
$$\phi(k) = \frac{1}{2}(\alpha-\gamma-2k-\pi). \tag{27}$$

Following the argument given in [21], we consider a vector $\mathbf{p}(k) = (p_1(k), p_2(k), p_3(k))$ in the three-dimensional parameter space defined by

$$\begin{aligned} p_1(k) &= p(k)\sin\theta(k)\cos\phi(k), \\ p_2(k) &= p(k)\sin\theta(k)\sin\phi(k), \\ p_3(k) &= p(k)\cos\theta(k). \end{aligned} \tag{28}$$

Let

$$\begin{aligned} \hat{\mathbf{e}}_1 &= (-\sin\gamma, -\cos\gamma, 0), \\ \hat{\mathbf{e}}_2 &= (\sin\frac{\beta}{2}\cos\gamma, -\sin\frac{\beta}{2}\sin\gamma, -\cos\frac{\beta}{2}), \\ \hat{\mathbf{e}}_3 &= (\cos\frac{\beta}{2}\cos\gamma, -\cos\frac{\beta}{2}\sin\gamma, \sin\frac{\beta}{2}). \end{aligned} \tag{29}$$

Using (23)-(27), it is easy to confirm the fact that

$$\mathbf{p}(k) \perp \hat{\mathbf{e}}_3 \quad \text{for all} \quad k \in [-\pi, \pi),$$

which implies that $\mathbf{p}(k)$ draws an orbit on a plane including the origin, whose normal vector is $\hat{\mathbf{e}}_3$ in the parameter space. On this orbital plane, we define the angle χ by $\cos\chi = \hat{\mathbf{p}}(k)\cdot\hat{\mathbf{e}}_1$, where $\hat{\mathbf{p}}(k) = \mathbf{p}(k)/p(k)$. Then we have the relations

$$\cos\chi = \frac{\sin(\beta/2)\cos\{(\alpha+\gamma-2k)/2\}}{\sqrt{1-\cos^2(\beta/2)\cos^2\{(\alpha+\gamma-2k)/2\}}}, \tag{30}$$
$$\sin\chi = \frac{\sin\{(\alpha+\gamma-2k)/2\}}{\sqrt{1-\cos^2(\beta/2)\cos^2\{(\alpha+\gamma-2k)/2\}}}. \tag{31}$$

Comparing (30) with (23) and (24), the equation of the orbit on the plane is determined of essentially the same form as reported in [21],

$$\tan\frac{p(k)}{2} = \tan\frac{\beta}{2}\frac{1}{\cos\chi}. \tag{32}$$

As pointed by [21], the integral with respect to the wave number k in (22) is mapped to the curvilinear integration along the orbit with respect to the angle χ through the relations (30) and (31), or their inverted forms

$$\cos\frac{1}{2}(\alpha+\gamma-2k) = \frac{\cos\chi}{\sqrt{1-\cos^2(\beta/2)\sin^2\chi}}, \tag{33}$$
$$\sin\frac{1}{2}(\alpha+\gamma-2k) = \frac{\sin\chi\sin(\beta/2)}{\sqrt{1-\cos^2(\beta/2)\sin^2\chi}}. \tag{34}$$

The Jacobian associated with the map $k \mapsto \chi$ is obtained as

$$J \equiv \left|\frac{dk}{d\chi}\right| = \frac{\sin(\beta/2)}{1-\cos^2(\beta/2)\sin^2\chi}. \tag{35}$$

From (24), we have

$$p(k) = 2\arccos\left\{\cos\frac{\beta}{2}\cos\frac{1}{2}(\alpha+\gamma-2k)\right\},$$

and then

$$\frac{dp(k)}{dk} = -2\cos\frac{\beta}{2}\sin\chi, \tag{36}$$

where the formula $(d/dx)\text{arccos}x = \mp 1/\sqrt{1-x^2}$ has been used. The long-time limit (22) of moments of pseudovelocity is now expressed as

$$\lim_{t\to\infty} \left\langle \left(\frac{X_t^{(j)}}{t}\right)^r \right\rangle = \sum_{m:0<m\leq j} I_m^{(j)}(r), \quad r = 1,2,3,\cdots, \tag{37}$$

where

$$\begin{aligned} I_m^{(j)}(r) &= \int_{-\pi}^{\pi} \frac{d\chi}{2\pi} \frac{\sin(\beta/2)}{1-\cos^2(\beta/2)\sin^2\chi} \\ &\times \left\{ |\hat{C}_m^{(j)}(\chi)|^2 + (-1)^r |\hat{C}_{-m}^{(j)}(\chi)|^2 \right\} \\ &\times \left(2m\cos\frac{\beta}{2}\sin\chi\right)^r \end{aligned} \tag{38}$$

with $\hat{C}_{\pm m}^{(j)}(\chi) \equiv C_{\pm m}^{(j)}(k(\chi))$.

C. Superposition of scaled Konno's density functions

In each integral $I_m^{(j)}(r)$, we change the variable of integral from χ to y by

$$y = 2m\cos\frac{\beta}{2}\sin\chi. \tag{39}$$

If we assume that by this change of variable $\hat{C}_m^{(j)}(\chi)$ is replaced by $c_m^{(j)}(y)$, the integral is written as

$$\begin{aligned} I_m^{(j)}(r) &= \frac{1}{2m}\int_{-\infty}^{\infty} dy\, y^r \mu\left(\frac{y}{2m};\cos\frac{\beta}{2}\right) \\ &\times \left\{ |c_m^{(j)}(y)|^2 + (-1)^r |c_{-m}^{(j)}(y)|^2 \right\}. \end{aligned} \tag{40}$$

Here $\mu(x;a)$ is given by (2), which is the density function first introduced by Konno to describe the limit distributions of the two-component one-dimensional quantum walks in his weak limit theorem [9, 10]. As a function of y, $|c_m^{(j)}(y)|^2$ is separated into an even-function part and an odd-function part. For positive values of m, let $\mathcal{M}_{\text{even}}^{(j,m)}(y/2m) =$ even-function part of $|c_m^{(j)}(y)|^2 + |c_{-m}^{(j)}(y)|^2$ and $\mathcal{M}_{\text{odd}}^{(j,m)}(y/2m) =$ odd-function part of $|c_m^{(j)}(y)|^2 - |c_{-m}^{(j)}(y)|^2$. Since $\mu(x;a)$ is an even function of x, (40) gives

$$\begin{aligned} I_m^{(j)}(2n) &= \frac{1}{2m}\int_{-\infty}^{\infty} dy\, y^{2n} \mu\left(\frac{y}{2m};\cos\frac{\beta}{2}\right) \\ &\times \mathcal{M}_{\text{even}}^{(j,m)}\left(\frac{y}{2m}\right), \\ I_m^{(j)}(2n-1) &= \frac{1}{2m}\int_{-\infty}^{\infty} dy\, y^{2n-1} \mu\left(\frac{y}{2m};\cos\frac{\beta}{2}\right) \\ &\times \mathcal{M}_{\text{odd}}^{(j,m)}\left(\frac{y}{2m}\right) \end{aligned} \tag{41}$$

for $n = 1,2,3,\cdots$. Then (37) implies that

$$\begin{aligned} &\lim_{t\to\infty} \left\langle \left(\frac{X_t^{(j)}}{t}\right)^r \right\rangle \\ &= \int_{-\infty}^{\infty} dy\, y^r \sum_{m:0<m\leq j} \frac{1}{2m}\mu\left(\frac{y}{2m};\cos\frac{\beta}{2}\right) \\ &\quad \times \mathcal{M}^{(j,m)}\left(\frac{y}{2m}\right) \end{aligned} \tag{42}$$

for $r = 1,2,3,\cdots$, where

$$\mathcal{M}^{(j,m)}(x) = \mathcal{M}_{\text{even}}^{(j,m)}(x) + \mathcal{M}_{\text{odd}}^{(j,m)}(x). \tag{43}$$

When j is a positive integer, (*i.e.*, $(2j+1)$ is odd), the integral

$$\begin{aligned} J^{(j)} &= \int_{-\infty}^{\infty} dy \sum_{m:0<m\leq j} \frac{1}{2m}\mu\left(\frac{y}{2m};\cos\frac{\beta}{2}\right) \\ &\times \mathcal{M}^{(j,m)}\left(\frac{y}{2m}\right) \end{aligned} \tag{44}$$

is generally less than one, since the contribution from the $m = 0$ mode is not included in the summation. The difference

$$\Delta^{(j)} = 1 - J^{(j)} \tag{45}$$

gives the weight of a point mass at $y = 0$ in the distribution.

The result is summarized as follows. The long-time limit of the pseudovelocity of $(2j+1)$-component quantum walk is described by the probability measure, which consists of the summation of appropriately scaled Konno's density functions with weight functions $\mathcal{M}^{(j,m)}(y/2m)$, and a point mass at the origin with weight $\Delta^{(j)}$, if the number of components $(2j+1)$ is odd, that is

$$\lim_{t\to\infty} \left\langle \left(\frac{X_t^{(j)}}{t}\right)^r \right\rangle = \int_{-\infty}^{\infty} dy\, y^r \nu^{(j)}(y), \quad r = 0,1,2,\cdots \tag{46}$$

with

$$\begin{aligned} \nu^{(j)}(y) &= \sum_{m:0<m\leq j} \frac{1}{2m}\mu\left(\frac{y}{2m};\cos\frac{\beta}{2}\right)\mathcal{M}^{(j,m)}\left(\frac{y}{2m}\right) \\ &+ \mathbf{1}_{\{(2j+1)\text{ is odd}\}}\Delta^{(j)}\delta(y). \end{aligned} \tag{47}$$

D. Polynomials $\mathcal{M}^{(j,m)}(x)$ representing parameter and initial-qubit dependence

Using the formulas given in Appendix C and the matrices $r^{(j)}$ in Appendix A, the weights $\mathcal{M}^{(j,m)}(x)$ and $\Delta^{(j)}$ in the limit distribution (47) are explicitly determined as follows for $j = 1/2, 1$ and $3/2$, $0 < m \leq j$. Set

$$\tau = \tan\frac{\beta}{2}. \tag{48}$$

For a complex number z, $\mathrm{Re}\{z\}$ denotes the real part of z.

$j = 1/2$ case (two-component model)

$$\mathcal{M}^{(1/2,1/2)}(x) = 1 + \mathcal{M}_1^{(1/2,1/2)} x, \tag{49}$$

with

$$\begin{aligned} \mathcal{M}_1^{(1/2,1/2)} &= -\{|q_{1/2}|^2 - |q_{-1/2}|^2\} \\ &\quad + 2\tau\,\mathrm{Re}\Big\{q_{1/2}\overline{q}_{-1/2}e^{-\mathrm{i}\gamma}\Big\}. \end{aligned} \tag{50}$$

When $\mathcal{M}_1^{(1/2,1/2)} = 0$ (resp. $\mathcal{M}_1^{(1/2,1/2)} \neq 0$), the limit distribution $\nu^{(1/2)}(y)$ is symmetric (resp. asymmetric) [9, 10, 21].

$j = 1$ case (three-component model)

$$\mathcal{M}^{(1,1)}(x) = \mathcal{M}_0^{(1,1)} + \mathcal{M}_1^{(1,1)} x + \mathcal{M}_2^{(1,1)} x^2, \tag{51}$$

with

$$\begin{aligned} \mathcal{M}_0^{(1,1)} &= \frac{1}{2}\{|q_1|^2 + 2|q_0|^2 + |q_{-1}|^2\} - \mathrm{Re}\Big\{q_1\overline{q}_{-1}e^{-2\mathrm{i}\gamma}\Big\}, \\ \mathcal{M}_1^{(1,1)} &= -\{|q_1|^2 - |q_{-1}|^2\} \\ &\quad + \sqrt{2}\tau\,\mathrm{Re}\Big\{(q_1\overline{q}_0 + q_0\overline{q}_{-1})e^{-\mathrm{i}\gamma}\Big\}, \\ \mathcal{M}_2^{(1,1)} &= \frac{1}{2}\{|q_1|^2 - 2|q_0|^2 + |q_{-1}|^2\} \\ &\quad - \sqrt{2}\tau\,\mathrm{Re}\Big\{(q_1\overline{q}_0 - q_0\overline{q}_{-1})e^{-\mathrm{i}\gamma}\Big\} \\ &\quad + (1 + 2\tau^2)\,\mathrm{Re}\Big\{q_1\overline{q}_{-1}e^{-2\mathrm{i}\gamma}\Big\}, \end{aligned} \tag{52}$$

and

$$\Delta^{(1)} = 1 - \left\{\mathcal{M}_0^{(1,1)} + \left(1 - \sin\frac{\beta}{2}\right)\mathcal{M}_2^{(1,1)}\right\}. \tag{53}$$

The condition that the limit distribution $\nu^{(1)}(y)$ is symmetric is given by $\mathcal{M}_1^{(1,1)} = 0$. Generally the point mass at the origin appears with the weight $\Delta^{(1)}$ in the limit distribution.

$j = 3/2$ case (four-component model)

$$\mathcal{M}^{(3/2,3/2)}(x) = \mathcal{M}_0^{(3/2,3/2)} + \mathcal{M}_1^{(3/2,3/2)} x + \mathcal{M}_2^{(3/2,3/2)} x^2 + \mathcal{M}_3^{(3/2,3/2)} x^3, \tag{54}$$

and

$$\mathcal{M}^{(3/2,1/2)}(x) = \mathcal{M}_0^{(3/2,1/2)} + \mathcal{M}_1^{(3/2,1/2)} x + \mathcal{M}_2^{(3/2,1/2)} x^2 + \mathcal{M}_3^{(3/2,1/2)} x^3, \tag{55}$$

with

$$\begin{aligned} \mathcal{M}_0^{(3/2,3/2)} &= \frac{1}{4}\Big\{|q_{3/2}|^2 + 3|q_{1/2}|^2 + 3|q_{-1/2}|^2 + |q_{-3/2}|^2\Big\} - \frac{\sqrt{3}}{2}\mathrm{Re}\Big\{(q_{3/2}\overline{q}_{-1/2} + q_{1/2}\overline{q}_{-3/2})e^{-2\mathrm{i}\gamma}\Big\}, \\ \mathcal{M}_1^{(3/2,3/2)} &= -\frac{3}{4}\Big\{|q_{3/2}|^2 + |q_{1/2}|^2 - |q_{-1/2}|^2 - |q_{-3/2}|^2\Big\} - \frac{3}{2}\tau\,\mathrm{Re}\Big\{q_{3/2}\overline{q}_{-3/2}e^{-3\mathrm{i}\gamma} - q_{1/2}\overline{q}_{-1/2}e^{-\mathrm{i}\gamma}\Big\} \\ &\quad + \frac{\sqrt{3}}{2}\tau\,\mathrm{Re}\Big\{(q_{3/2}\overline{q}_{1/2} + q_{-1/2}\overline{q}_{-3/2})e^{-\mathrm{i}\gamma}\Big\} + \frac{\sqrt{3}}{2}\mathrm{Re}\Big\{(q_{3/2}\overline{q}_{-1/2} - q_{1/2}\overline{q}_{-3/2})e^{-2\mathrm{i}\gamma}\Big\}, \\ \mathcal{M}_2^{(3/2,3/2)} &= \frac{3}{4}\Big\{|q_{3/2}|^2 - |q_{1/2}|^2 - |q_{-1/2}|^2 + |q_{-3/2}|^2\Big\} - \sqrt{3}\tau\,\mathrm{Re}\Big\{(q_{3/2}\overline{q}_{1/2} - q_{-1/2}\overline{q}_{-3/2})e^{-\mathrm{i}\gamma}\Big\} \\ &\quad + \frac{\sqrt{3}}{2}(1 + 2\tau^2)\,\mathrm{Re}\Big\{(q_{3/2}\overline{q}_{-1/2} + q_{1/2}\overline{q}_{-3/2})e^{-2\mathrm{i}\gamma}\Big\}, \\ \mathcal{M}_3^{(3/2,3/2)} &= -\frac{1}{4}\Big\{|q_{3/2}|^2 - 3|q_{1/2}|^2 + 3|q_{-1/2}|^2 - |q_{-3/2}|^2\Big\} + \frac{1}{2}\tau(3 + 4\tau^2)\,\mathrm{Re}\Big\{q_{3/2}\overline{q}_{-3/2}e^{-3\mathrm{i}\gamma}\Big\} \\ &\quad - \frac{3}{2}\tau\,\mathrm{Re}\Big\{q_{1/2}\overline{q}_{-1/2}e^{-\mathrm{i}\gamma}\Big\} + \frac{\sqrt{3}}{2}\tau\,\mathrm{Re}\Big\{(q_{3/2}\overline{q}_{1/2} + q_{-1/2}\overline{q}_{-3/2})e^{-\mathrm{i}\gamma}\Big\} \\ &\quad - \frac{\sqrt{3}}{2}(1 + 2\tau^2)\,\mathrm{Re}\Big\{(q_{3/2}\overline{q}_{-1/2} - q_{1/2}\overline{q}_{-3/2})e^{-2\mathrm{i}\gamma}\Big\}, \end{aligned} \tag{56}$$

and with

$$\begin{aligned} \mathcal{M}_0^{(3/2,1/2)} &= \frac{1}{4}\Big\{3|q_{3/2}|^2 + |q_{1/2}|^2 + |q_{-1/2}|^2 + 3|q_{-3/2}|^2\Big\} + \frac{\sqrt{3}}{2}\mathrm{Re}\Big\{(q_{3/2}\overline{q}_{-1/2} + q_{1/2}\overline{q}_{-3/2})e^{-2\mathrm{i}\gamma}\Big\}, \\ \mathcal{M}_1^{(3/2,1/2)} &= -\frac{1}{4}\Big\{3|q_{3/2}|^2 - 5|q_{1/2}|^2 + 5|q_{-1/2}|^2 - 3|q_{-3/2}|^2\Big\} + \frac{9}{2}\tau\,\mathrm{Re}\Big\{q_{3/2}\overline{q}_{-3/2}e^{-3\mathrm{i}\gamma}\Big\} \end{aligned}$$

$$
\begin{aligned}
&-\frac{1}{2}\tau\,\mathrm{Re}\Big\{q_{1/2}\overline{q}_{-1/2}e^{-\mathrm{i}\gamma}\Big\}+\frac{\sqrt{3}}{2}\tau\,\mathrm{Re}\Big\{(q_{3/2}\overline{q}_{1/2}+q_{-1/2}\overline{q}_{-3/2})e^{-\mathrm{i}\gamma}\Big\}\\
&-\frac{3\sqrt{3}}{2}\mathrm{Re}\Big\{(q_{3/2}\overline{q}_{-1/2}-q_{1/2}\overline{q}_{-3/2})e^{-2\mathrm{i}\gamma}\Big\},\\
\mathcal{M}_2^{(3/2,1/2)} \;=\;& -\frac{3}{4}\Big\{|q_{3/2}|^2-|q_{1/2}|^2-|q_{-1/2}|^2+|q_{-3/2}|^2\Big\}+\sqrt{3}\tau\,\mathrm{Re}\Big\{(q_{3/2}\overline{q}_{1/2}-q_{-1/2}\overline{q}_{-3/2})e^{-\mathrm{i}\gamma}\Big\}\\
&-\frac{\sqrt{3}}{2}(1+2\tau^2)\,\mathrm{Re}\Big\{(q_{3/2}\overline{q}_{-1/2}+q_{1/2}\overline{q}_{-3/2})e^{-2\mathrm{i}\gamma}\Big\},\\
\mathcal{M}_3^{(3/2,1/2)} \;=\;& \frac{3}{4}\Big\{|q_{3/2}|^2-3|q_{1/2}|^2+3|q_{-1/2}|^2-|q_{-3/2}|^2\Big\}-\frac{3}{2}\tau(3+4\tau^2)\,\mathrm{Re}\Big\{q_{3/2}\overline{q}_{-3/2}e^{-3\mathrm{i}\gamma}\Big\}\\
&+\frac{9}{2}\tau\,\mathrm{Re}\Big\{q_{1/2}\overline{q}_{-1/2}e^{-\mathrm{i}\gamma}\Big\}-\frac{3\sqrt{3}}{2}\tau\,\mathrm{Re}\Big\{(q_{3/2}\overline{q}_{1/2}+q_{-1/2}\overline{q}_{-3/2})e^{-\mathrm{i}\gamma}\Big\}\\
&+\frac{3\sqrt{3}}{2}(1+2\tau^2)\,\mathrm{Re}\Big\{(q_{3/2}\overline{q}_{-1/2}-q_{1/2}\overline{q}_{-3/2})e^{-2\mathrm{i}\gamma}\Big\}. \qquad (57)
\end{aligned}
$$

If and only if $\mathcal{M}_1^{(3/2,3/2)}=\mathcal{M}_3^{(3/2,3/2)}=0$ and $\mathcal{M}_1^{(3/2,1/2)}=\mathcal{M}_3^{(3/2,1/2)}=0$, the limit distribution $\nu^{(3/2)}(y)$ is symmetric.

These results imply that $\mathcal{M}^{(j,m)}(x)$ are polynomials of x of degree $2j$ and the coefficients $\mathcal{M}_k^{(j,m)}, k=0,1,\cdots,2j$ depend on β and γ through the functions $\tau=\tan(\beta/2)$ and $e^{-\mathrm{i}\gamma}$, but they do not on α. It should be noted that their dependence on initial qubit (1) is complicated. In other words, the limit distribution of pseudovelocity of quantum walk is very sensitive to changes of initial qubit.

V. COMPARISON WITH COMPUTER SIMULATIONS AND CONCLUDING REMARKS

In order to demonstrate the validity of the above results, here we show comparison with computer simulation results. In the following figures, Figs.2-4, the scattering thin lines indicate the distribution of X_t/t at time step $t=100$ obtained by computer simulation and the thick lines the limit distribution functions $\nu^{(j)}(y)$ given in the previous section.

Two-component model

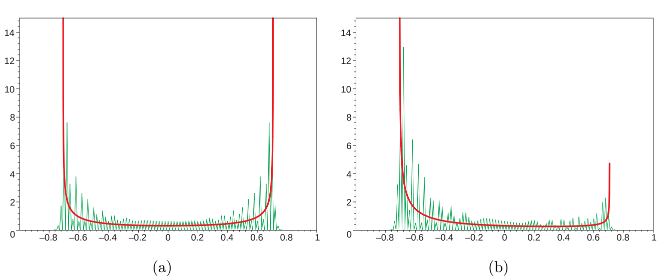

FIG. 2: Comparison between simulation results and limit distributions for the two-component model. (a) Symmetric and (b) asymmetric cases.

The result (49) with (50) is completely identified with the previous results [9, 10, 21]. Here we put $(\alpha,\beta,\gamma)=(0,-3\pi/2,\pi)$. Then we have

$$R^{(1/2)}=\frac{\mathrm{i}}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}, \qquad (58)$$

which is the Hadamard matrix multiplied by i. (Remark that the factor i is irrelevant for limit distribution, but by this factor $R^{(1/2)}$ is in SU(2), see [21].) When we choose the initial qubit as ${}^t\phi_0=(1+\mathrm{i},1-\mathrm{i})/2$, the limit distribution of pseudovelocity is symmetric as shown by Fig.2 (a), but when we choose ${}^t\phi_0=(1+\mathrm{i},1+\mathrm{i})/2$, only changing the sign of imaginary part of the second component, the limit distribution becomes asymmetric as shown by Fig. 2 (b). When $(\alpha,\beta,\gamma)=(0,-3\pi/2,\pi)$, the former initial qubit satisfies the condition $\mathcal{M}_1^{(1/2,1/2)}=0$, but the latter does not, where $\mathcal{M}_1^{(1/2,1/2)}$ is given by (50). The shape of limit distribution function is very sensitive to changes of initial qubit.

Three-component model

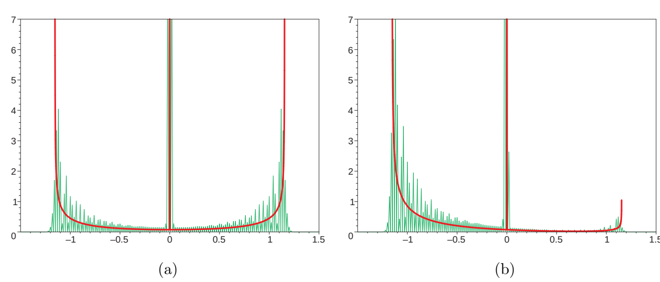

FIG. 3: Comparison between simulation results and limit distributions for the three-component model. (a) Symmetric and (b) asymmetric cases. The perpendicular thick lines at the origin indicate Dirac's delta functions.

If we set $(\alpha,\beta,\gamma)=(0,\arccos(-1/3),\pi)$, the three-component quantum coin will be

$$R^{(1)} = \frac{1}{3}\begin{pmatrix} -1 & -2 & -2 \\ -2 & -1 & 2 \\ -2 & 2 & -1 \end{pmatrix}. \tag{59}$$

Remark that it is similar to the Grover matrix [12], but it is not the same. Figure 3 shows the comparison of simulation results and limit distributions for (a) ${}^t\phi_0 = (1-\mathrm{i}, 1+\mathrm{i}, 1-\mathrm{i})/\sqrt{6}$, which gives symmetric distribution, and for (b) ${}^t\phi_0 = (1-\mathrm{i}, 1-\mathrm{i}, 1-\mathrm{i})/\sqrt{6}$, which gives asymmetric distribution, respectively. It is readily checked that the case (a) satisfies the condition $\mathcal{M}_1^{(1,1)} = 0$ for symmetric distribution. In the three-component model, Dirac's delta-function-type peak at the origin is usually observed in simulation.

Four-component model

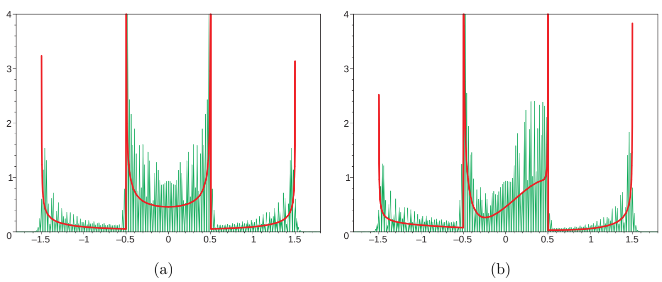

FIG. 4: Comparison between simulation results and limit distributions for the four-component model. (a) Symmetric and (b) asymmetric cases.

We set $(\alpha, \beta, \gamma) = (0, 2\pi/3, \pi)$ for the four-component model, which corresponds to choosing the quantum coin as

$$R^{(3/2)} = \frac{\mathrm{i}}{8}\begin{pmatrix} 1 & 3 & 3\sqrt{3} & 3\sqrt{3} \\ 3 & 5 & \sqrt{3} & -3\sqrt{3} \\ 3\sqrt{3} & \sqrt{3} & -5 & 3 \\ 3\sqrt{3} & -3\sqrt{3} & 3 & -1 \end{pmatrix}. \tag{60}$$

If we assume the initial qubit as

$$\phi_0 = \frac{1}{2\sqrt{5}}\begin{pmatrix} 1+3\mathrm{i} \\ 0 \\ 0 \\ -3+\mathrm{i} \end{pmatrix} \text{ and } \phi_0 = \frac{1}{2\sqrt{5}}\begin{pmatrix} 1+3\mathrm{i} \\ 0 \\ 0 \\ -3-\mathrm{i} \end{pmatrix}, \tag{61}$$

the distributions are determined as shown in Fig. 4 (a) and Fig. 4 (b), respectively.

We observe oscillatory behavior of distribution functions of X_t/t in computer simulations. In general, as the time step t increases, the frequency of oscillation becomes higher. But the convergence of any moments given by (46) means that, if we smear out the oscillatory behavior, the averaged lines of distribution functions will be well-described by the limit distribution functions (47), which is the fact demonstrated by the above figures.

Now we discuss possible future problems related with the present work. Inui and Konno [27] and Inui *et al.* [28] introduced a one-dimensional three-component quantum walk and showed that a kind of localization phenomenon occurs in their model by calculating the long-time distribution of walker's position X_t. They claimed that such a localization phenomenon results in a point mass at the origin, represented by Dirac's delta function, in the limit distribution of X_t/t. Though their model associated with the Grover matrix does not belong to our family of models, the structure of limit distribution obtained in our three-component model ($j = 1$ case) (47) with $j = m = 1$ and with (51) is very similar to the limit distribution function of X_t/t, given by Eq.(16) in [28]. Then the present work suggests that such a localization phenomenon is universal for the models, in which there is a positive probability for walker to stay at the same position in each step. Systematic study of localization phenomena in quantum-walk models will be an interesting future problem. Venegas-Andraca *et al.* [29] reported quantum-walk models with entangle coins, where a variety of distributions of walker's position with multi-peak zones are plotted in figures. They constructed quantum coins for multi-component qubits by considering tensor products of the basic two-component quantum coins. In other words, using tensor products of $j = 1/2$ states with $m = \pm 1/2$, the quantum states with higher values of $m = \pm 1, \pm 3/2, \cdots$, are introduced in the models. On the other hands, in our family of models, by raising the value of j the quantum states with higher values of m are systematically included in the models, and thus multi-peak structures are controlled by the value of j. We have used the Wigner formula, which gives irreducible representation of the rotation group. In general, in order to decompose the tensor product space into irreducible representations, we need to use a procedure, *e.g.*, the highest weight procedure [25]. Further study on the relationship between the present work and [29] will be interesting. In the present paper, we gave the explicit expressions of $\mathcal{M}^{(j,m)}(x)$ for $j = 1/2, 1$ and $3/2$. Here we gave only key formulas in Appendix C for calculation of them, but the present result implies that $\mathcal{M}^{(j,m)}(x)$ are generally given by polynomials. Reminding the fact that the orthogonal polynomials (e.g. Hermite, Legendre, and Laguerre polynomials) have played very important roles in quantum mechanics, we hope that further study of $\mathcal{M}^{(j,m)}$ is a promising subject in the field of quantum walks. As reported in [11, 18, 29, 30], multi-component models have been studied to simulate quantum walks on the plane, in the higher-dimensional lattices $\mathbf{Z}^d$, or on general graphs. The present work suggests that the group-theoretical investigation will be useful to perform systematic study of such extended models of quantum walks and quantum processes.

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APPENDIX A: THE MATRICES $r^{(j)}(\beta)$ FOR $j = 1/2, 1, 3/2$

The explicit expressions of $r^{(j)}(\beta)$ are readily derived from the Wigner formula (7) as follows for $j = 1/2, 1, 3/2$. Let $c = \cos(\beta/2)$, $s = \sin(\beta/2)$. Then

$$r^{(1/2)}(\beta) = \begin{pmatrix} c & -s \\ s & c \end{pmatrix}, \tag{A1}$$

$$r^{(1)}(\beta) = \begin{pmatrix} c^2 & -\sqrt{2}cs & s^2 \\ \sqrt{2}cs & 2c^2-1 & -\sqrt{2}cs \\ s^2 & \sqrt{2}cs & c^2 \end{pmatrix}, \tag{A2}$$

$$r^{(3/2)}(\beta) = \begin{pmatrix} c^3 & -\sqrt{3}c^2 s & \sqrt{3}cs^2 & -s^3 \\ \sqrt{3}c^2 s & -2cs^2+c^3 & s^3-2c^2 s & \sqrt{3}cs^2 \\ \sqrt{3}cs^2 & -s^3+2c^2 s & -2cs^2+c^3 & -\sqrt{3}c^2 s \\ s^3 & \sqrt{3}cs^2 & \sqrt{3}c^2 s & c^3 \end{pmatrix}. \tag{A3}$$

APPENDIX B: PROOF OF EQUATIONS (18) WITH (19)

By definitions (5), (13) with $S^{(j)}(k) = R^{(j)}(-2k, 0, 0)$, $V^{(j)}(k) = R^{(j)}(\alpha - 2k, \beta, \gamma)$. Then it is enough to prove the equality

$$R^{(j)}(\alpha, \beta, \gamma) = R^{(j)}(\phi, \theta, 0) R^{(j)}(-p, 0, 0) [R^{(j)}(\phi, \theta, 0)]^\dagger \tag{B1}$$

with relations

$$\frac{1}{2}(\alpha - \gamma) = \phi + \frac{\pi}{2}, \quad \tan\frac{1}{2}(\alpha + \gamma) = -\tan\frac{p}{2}\cos\theta, \quad \sin\frac{\beta}{2} = \sin\frac{p}{2}\sin\theta. \tag{B2}$$

The equality (B1) is a matrix representation of the equality which will hold among the rotations

$$\hat{R}(\alpha, \beta, \gamma) = \hat{R}(\phi, \theta, 0)\hat{R}(-p, 0, 0)[\hat{R}(\phi, \theta, 0)]^\dagger. \tag{B3}$$

Since rotation matrices defined by (5) with $j = 1/2, 1, 3/2, \cdots$ are faithful representations of rotations, it may be enough to prove the equality (B1) for the simplest case, $j = 1/2$, since it implies (B3).

By direct calculation, we have

$$\begin{aligned} & R^{(1/2)}(\phi, \theta, 0) R^{(1/2)}(-p, 0, 0) [R^{(1/2)}(\phi, \theta, 0)]^\dagger \\ = & \begin{pmatrix} e^{-\mathrm{i}\phi/2}\cos(\theta/2) & -e^{-\mathrm{i}\phi/2}\sin(\theta/2) \\ e^{\mathrm{i}\phi/2}\sin(\theta/2) & e^{\mathrm{i}\phi/2}\cos(\theta/2) \end{pmatrix} \begin{pmatrix} e^{\mathrm{i}p/2} & 0 \\ 0 & e^{-\mathrm{i}p/2} \end{pmatrix} \begin{pmatrix} e^{\mathrm{i}\phi/2}\cos(\theta/2) & e^{-\mathrm{i}\phi/2}\sin(\theta/2) \\ -e^{\mathrm{i}\phi/2}\sin(\theta/2) & e^{-\mathrm{i}\phi/2}\cos(\theta/2) \end{pmatrix} \\ = & \begin{pmatrix} \cos(p/2) + \mathrm{i}\sin(p/2)\cos\theta & \mathrm{i}\sin(p/2)\sin\theta e^{-\mathrm{i}\phi} \\ \mathrm{i}\sin(p/2)\sin\theta e^{\mathrm{i}\phi} & \cos(p/2) - \mathrm{i}\sin(p/2)\cos\theta \end{pmatrix}. \end{aligned} \tag{B4}$$

Comparing it with

$$R^{(1/2)}(\alpha, \beta, \gamma) = \begin{pmatrix} e^{-\mathrm{i}(\alpha+\gamma)/2}\cos(\beta/2) & -e^{-\mathrm{i}(\alpha-\gamma)/2}\sin(\beta/2) \\ e^{\mathrm{i}(\alpha-\gamma)/2}\sin(\beta/2) & e^{\mathrm{i}(\alpha+\gamma)/2}\cos(\beta/2) \end{pmatrix},$$

we have the equations

$$\begin{aligned} \cos\frac{p}{2} &= \cos\frac{\beta}{2}\cos\frac{1}{2}(\alpha+\gamma), \\ \sin\frac{p}{2}\cos\theta &= -\cos\frac{\beta}{2}\sin\frac{1}{2}(\alpha+\gamma), \\ \sin\frac{p}{2}\sin\theta\sin\phi &= -\sin\frac{\beta}{2}\cos\frac{1}{2}(\alpha-\gamma), \\ \sin\frac{p}{2}\sin\theta\cos\phi &= \sin\frac{\beta}{2}\sin\frac{1}{2}(\alpha-\gamma), \end{aligned} \tag{B5}$$

from which (B2) is derived.

APPENDIX C: FORMULAS

Inserting (6) with (7) into (21) and taking square of the complex variable, we have the expression

$$|C_m^{(j)}(k)|^2 = \sum_{m_1=-j}^{j}\sum_{m_2=-j}^{j} q_{m_1}\overline{q}_{m_2} e^{\mathrm{i}(m_1-m_2)\phi(k)} \times \sum_{\ell_1}\sum_{\ell_2}\Gamma(j, m_1, m, \ell_1)\Gamma(j, m_2, m, \ell_2) \times \left(\cos\frac{\theta(k)}{2}\right)^{4j+m_1+m_2-2m-2\ell_1-2\ell_2}$$

$$\times \left(\sin \frac{\theta(k)}{2}\right)^{2\ell_1+2\ell_2+2m-m_1-m_2}. \tag{C1}$$

From (25)-(27), the following relations are derived,

$$\cos\theta(k) = -\cos\frac{\beta}{2}\sin\chi,$$
$$\sin\theta(k)e^{\mathrm{i}\phi(k)} = \left(\sin\frac{\beta}{2}\sin\chi - \mathrm{i}\cos\chi\right)e^{-\mathrm{i}\gamma}. \tag{C2}$$

Then, through the change of variable (39), we have

$$\cos^2\frac{\theta(k)}{2} = \frac{1}{2}\left(1-\frac{y}{2m}\right),$$
$$\sin^2\frac{\theta(k)}{2} = \frac{1}{2}\left(1+\frac{y}{2m}\right),$$
$$\sin\frac{\theta(k)}{2}\cos\frac{\theta(k)}{2}e^{\mathrm{i}\phi(k)}$$
$$= \frac{1}{2}\left\{\frac{y}{2m}\tan\frac{\beta}{2} - \mathrm{i}\sqrt{1-\left(\frac{y}{2m}\right)^2\sec^2\frac{\beta}{2}}\right\}e^{-\mathrm{i}\gamma}. \tag{C3}$$

By (C3) we can perform the transformations $|C_m^{(j)}(k)|^2 \mapsto |\hat{C}_m^{(j)}(\chi)|^2 \mapsto |c_m^{(j)}(y)|^2$, and $\mathcal{M}^{(j,m)}(y/2m)$'s are obtained.

In order to calculate (53), we have used the following integral formulas,

$$\int_0^{2\cos(\beta/2)} \frac{1}{\sqrt{\cos^2(\beta/2)-(y/2)^2}}dy = \pi,$$
$$\int_0^{2\cos(\beta/2)} \frac{1}{\{1-(y/2)^2\}\sqrt{\cos^2(\beta/2)-(y/2)^2}}dy$$
$$= \frac{\pi}{\sin(\beta/2)}. \tag{C4}$$

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